Numerical investigation of single bubble dynamics in liquid sodium pool

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Abstract. The single gas bubble rise dynamics in liquid sodium/sodium-potassium alloy (NaK) pool due to entrainment of argon cover gas/non-condensable fission gas (xenon) have received considerable attention in the safe operation of Sodium-cooled Fast Reactor (SFR). Numerical simulation of single bubble dynamics in liquid sodium/NaK pool is an essential intermediate step for the evaluation of rise velocity and shape changes, which are of utmost importance in areas of reactor safety concerned with source term evaluation and cover gas purification. The interFoam solver of OpenFOAM package is used to evaluate inert gas bubble rise dynamics in stagnant liquid metal pool of sodium and NaK. The governing equations are discretized and solved using the Volume of Fluid (VOF) based solver available in OpenFOAM with appropriate initial and boundary conditions. The VOF module of the solver is validated against numerical benchmark data and experimental results available in literature. The bubble dynamics in liquid sodium/NaK pool are studied in terms of trajectory, shape and rise velocity for diameters ranging from 10 to 20 mm, domain aspect ratios and for different gas-liquid systems. The study shows that the bubble rise velocity increases with diameter for liquid sodium systems. The rise behavior of single inert gas bubble in liquid water and sodium pool are compared. The study supports the use of air-water system as a simulant for studying bubble dynamics in liquid sodium systems as suggested by other researchers. The study is very useful and forms an intermediate step towards the development of an OpenFOAM based computational framework to analyze heat and mass transfer from single bubble rising in liquid sodium pool for reactor safety studies.

Keywords. Bubble rise velocity; sodium; OpenFOAM.

1. Introduction

In Sodium-cooled Fast Reactors (SFRs), bubbles can result from entrainment of argon cover gas and non-condensable fission gas (xenon) within the sodium/sodium-potassium alloy (NaK) pool and also from sodium boiling following a flow/power transient [1]. The areas of reactor safety concerned with radioactive source term evaluation due to xenon bubble transport in sodium pool [2] and argon cover gas purification in sodium/NaK bubbler [3] is highly dependent on the bubble dynamic parameters such as rise velocity, shape and path. The rise velocity is an important parameter which limits the heat and mass transfer phenomena from rising bubbles in liquid sodium pool of SFR. One very fundamental study to be carried out towards this understanding is the rising and deforming of a single inert gas bubble in stagnant sodium/NaK pool. The single bubble dynamics in liquid pool is a function of bubble physical characteristics, properties of gas-liquid system and operating conditions. The knowledge of single bubble rise

dynamics forms an intermediate step towards the evaluation of complex heat and mass transport phenomena associated with SFR safety.

Numerous experiments [4] have been carried out to understand single air bubble dynamics in transparent liquids, especially water. Experimentally single gas bubbles can be generated using low gas injection rates. Experimental studies on bubble dynamics in transparent systems are measured using optical methods, often an imaging technique with a high speed camera. However, limitations in measurement techniques for opaque liquids reduced the bubble dynamic experiment capabilities in liquid metals (e.g., liquid sodium, NaK). The measurement techniques used for gas-liquid metal flows can be classified as invasive techniques (use of electrical resistivity, electrical capacitance, optical fiber, acoustic probes) or non-invasive techniques such as soft field tomography (use of acoustic, ultrasonic, electrical or magnetic signals) and hard field tomography (use of X-rays, neutron beams and gamma-rays). The X-ray attenuation techniques have been employed to view deep into the non-transparent liquid metal systems of GaInSn, iron and steel [5–7].

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The development of Computational Fluid Dynamics (CFD) technology has provided a convenient, effective and inexpensive tool to study bubble dynamics. This represents a complement to experimental measurements and provides better physical understanding of the phenomenon. Several numerical studies have been carried out to date to understand single bubble rise dynamics in stagnant liquids [8–15]. In source term evaluation studies related to SFR, single bubble dynamics in sodium pool is typically studied for a bubble size range from 10 mm to 30 mm [2, 16, 17] based on the maximum stable bubble size evaluated from fluid properties. However, based on experimental observations the bubble size is between 11 mm and 23 mm for SFR source term studies [18]. The fluid properties and experimental observations from earlier studies suggest a typical bubble size of 20 mm for SFR studies. Until now, theoretical research of the single bubble dynamics in liquid sodium pool were studied using correlations available in literature for bubble terminal velocity [19] or solving the equation of motion in terms of inertia, buoyancy and drag force [16].

In the present study, interFoam solver of Open Field Operation and Manipulation (OpenFOAM) is used to investigate the rise dynamics of single inert gas bubble in liquid sodium/NaK pool. The interFoam module used in the present study is verified and validated with numerical benchmarks and experimental correlations available in literature respectively for single bubble dynamics. Grid independence study is carried out to find the appropriate mesh size required for simulating inert bubble rise in liquid sodium. The bubble dynamics in liquid sodium is studied for various domain Aspect Ratio ($AR = \text{Height/Width}$), fluids and range of bubble diameters to understand their influence on bubble behavior. The present study is an intermediate step towards development of an OpenFOAM based computational framework to analyze heat and mass transfer from single bubble rising in liquid sodium pool for reactor safety studies.

2. Physical description of problem

The numerical investigation of single bubble (fluid 2) dynamics in liquid sodium (fluid 1) pool is carried out in a rectangular domain as shown in figure 1. Initially, the spherical bubble of diameter d_B is positioned at an elevation of $0.5 d_B$ from the bottom wall, along the central vertical axis. The gravitational acceleration of 9.81 m/s^2 is considered for the study. The present study considers thermal equilibrium between the gas bubble and liquid pool. The different parameters that affect the bubble dynamics are bubble diameter, domain Aspect Ratio ($AR = \text{Height/Width}$) and fluids. Hence the present study focuses on parametric studies to evaluate their influence.

3. Computational method

The rise of an inert gas bubble in liquid sodium pool is numerically investigated using the interFoam [20] solver available in an open source CFD package, OpenFOAM [21] version 3.0.0.

3.1 Governing equations

The governing conservation equations for mass, momentum and phase fraction are given below.

Continuity equation

$$\nabla \cdot \vec{u} = 0 \quad (1)$$

where, the mixed velocity is given by,

$$\vec{u} = \alpha_1 \vec{u}_1 + (1 - \alpha_1) \vec{u}_2 \quad (2)$$

The volume fraction of fluid 1

$$\alpha_1 = \begin{cases} 1 & \text{in fluid 1} \\ 0 & \text{in fluid 2} \\ 0 < \alpha_1 < 1 & \text{at the interface} \end{cases} \quad (3)$$

Momentum equation

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p_{rgh} + \nabla \cdot \left[\mu (\nabla \vec{u} + (\nabla \vec{u})^T) \right] - \vec{g} \cdot \vec{x} \nabla \rho + \sigma \kappa \nabla \alpha_1 \quad (4)$$

where, p_{rgh} is pseudo hydrostatic (dynamic) pressure, $\vec{x}$ is position vector, $\vec{g}$ is gravitational acceleration and σ is surface tension. The transport properties of mixed fluid, density ρ and viscosity μ are evaluated from the volume fraction weighted transport properties of two fluids.

$$\rho = \alpha_1 \rho_1 + (1 - \alpha_1) \rho_2 \quad (5)$$

$$\mu = \alpha_1 \mu_1 + (1 - \alpha_1) \mu_2 \quad (6)$$

$$p_{rgh} = p - \rho \vec{g} \cdot \vec{x} \quad (7)$$

Volume fraction equation for phase 1 [11]

$$\frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\vec{u} \alpha_1) + \nabla \cdot [\vec{u}_r \alpha_1 (1 - \alpha_1)] = 0 \quad (8)$$

where, the relative velocity between phases 1 and 2 is

$$\vec{u}_r = \vec{u}_1 - \vec{u}_2 \quad (9)$$

curvature of the interface is given by,

$$\kappa = -\nabla \cdot \hat{n} = -\nabla \cdot \left(\frac{\nabla \alpha_1}{|\nabla \alpha_1|} \right) \quad (10)$$

where, $\hat{n}$ is the interface unit normal vector

Figure 1. Computational domain.

3.2 Boundary conditions

The bottom and side walls are assigned no-slip boundary condition. The velocity is set to zero, the gradient of volume fraction of fluid 1 in the direction normal to wall boundary is also set to zero. The gradient of pressure normal to the wall boundary is calculated based on the velocity boundary condition predicted boundary flux (ϕ). The top boundary is free to the atmosphere and permits both inflow and outflow. Hence, a mixed boundary condition is used for the top boundary. The gradient of fluid 1 volume fraction in the direction normal to the top boundary is set to zero for outflow and for inflow, fluid 1 volume fraction is unity. The gradient of velocity in the direction normal to the top boundary is set to zero for outflow ($\phi > 0$) and velocity is set to zero for inflow ($\phi < 0$). The static pressure at the top boundary is obtained by subtracting the dynamic pressure from the specified total pressure.

3.3 Solution method

The interFoam solver uses Volume of Fluid (VOF) method [22] with surface compression [23] approach to solve the governing conservation equations. The details of the logic used for solving, algorithm of interFoam solver and discretization of governing equations have been described in detail by Klostermann *et al* [11].

3.3a Discretization details: Spatial discretization is carried out using finite volume Gaussian integration method and the implicit Euler method is used for temporal discretization. The interpolation scheme used for convective term in the momentum equation is limited linear. The interpolation scheme used for first and second convective terms in phase fraction equation are van Leer scheme [24] and a specialized interface compression scheme to gain smoother

interfaces. Multi-dimensional Universal Limiter for Explicit Solution (MULES) method is used to maintain boundedness of the volume fraction for solving volume fraction transport equation [21].

3.3b Solution algorithm: The algorithm used for pressure velocity coupling is PIMPLE (merged Pressure Implicit with Splitting of Operator (PISO) and Semi Implicit Method for Pressure Linked Equations (SIMPLE) algorithm) with three correction steps for pressure and two sub-cycles for the correction of the interface [21]. The PIMPLE algorithm has two loops, inner and outer [25]. In the outer loop all equations are solved while in the inner loop only continuity equation is solved. The pressure equation is solved in the outer loop for three correction steps to get time accuracy. The number of loops over the fluid 1 volume fraction is one for transient flow and the number of sub-cycles fluid 1 volume fraction is calculated is two. Conservative compression is used for compression term in the volume fraction equation. The equations solved are the pressure correction, the first pressure loop, the second and last pressure loops and the velocity equation. The solvers used are Preconditioned Bi-Conjugate Gradient (PBiCG) with Diagonal Incomplete-Lower Upper (DILU) preconditioner for velocity equation containing asymmetric matrices and the diagonal incomplete Cholesky (DIC) preconditioned CG for the pressure [21] equations containing symmetric matrices.

3.3c Computational details: The machine used for computation is Intel Core 2 Duo @ 2.4 GHz and 4 GB of RAM running on Ubuntu 14.04 OS. The typical computational time for a 20 mm argon bubble rising in a rectangular domain of liquid sodium is 4 days for a grid size of 544×544 .

3.4 Post processing

The post processing is carried out using the Swiss Army Knife for Foam (swak4Foam) toolbox. The toolbox allows user to put some conditions on the data extracted and also specify expressions involving the fields. The parameters evaluated using swak4Foam in the present study are the center of mass position coordinates of the bubble and the bubble rise velocity in y direction [26]. The center of mass position coordinates of the bubble is evaluated using the following equation.

$$\vec{X}_c = \int_{\Omega_1 \cap \Omega_2} \frac{\alpha_1 \vec{x}_c dA}{\alpha_1 dA} \quad (11)$$

where $\vec{x}_c = (x_c, y_c)$ is the center of mass position of an individual cell in the computational mesh. The average bubble rise velocity is obtained from ratio of axial displacement of center of mass to the rise time at any instant.

The bubble rise velocity in y direction is given as:

$$U_y = \frac{\int_{\Omega_1 \cap \Omega_2} \frac{\alpha_1 u_y dA}{\alpha_1 dA}}{\int_{\Omega_1 \cap \Omega_2} dA} \quad (12)$$

Where u_y is the velocity in y -direction in an individual cell of the computational mesh. The terminal rise velocity is obtained by averaging the values of rise velocity which does not change with time [26].

4. Validation

The interFoam solver used in the present study is verified against numerical benchmark results for rising bubble case. The solver is also validated against experimental data available in literature. The details of numerical verification and experimental validation of solver is described in the following section.

4.1 Numerical verification of solver

The verification of VOF module of interFoam solver is carried out using numerical benchmark results available in literature [27] for single bubble dynamics. The domain considered for verification is a rectangular space of 2 m height and 1 m width, which is filled with fluid 1. A bubble containing fluid 2 is positioned in the domain at an elevation of 0.5 m above the bottom wall along the central axis. Numerical verification is carried out for $d_B = 0.5$ m using the fluid properties in each of the benchmark cases as shown in table 1. The boundary conditions are *no slip* ($\vec{u} = 0$) for the top and bottom boundaries and *slip* for side boundaries. The gradient of volume fraction of fluid 1 in the direction normal to top, bottom and side boundaries are set to zero. The velocity is set to zero for top and bottom boundaries. The slip boundary conditions for the side wall sets the normal velocity component zero and the gradient of tangential velocity component in the normal direction as zero. The gradient of dynamic pressure in the direction normal to bottom and side boundaries are set to zero and constant pressure is set for the top boundary.

The quantitative benchmarks for bubble rise cases 1 and 2 were generated using numerical codes by Hysing *et al* [27]. The numerical codes used were TP2D, FreeLIFE and MooNMD. The TP2D code (Transport Phenomena in 2D) and FreeLIFE (Free-surface LIBrary of Finite Element) are

based on finite element discretizations with level set method to track the location of the interface between two fluids. MooNMD (Mathematics and object-oriented Numerics in MagDeburg) is also based on finite element discretization and treats incompressible two phase flows using the arbitrary Lagrangian Eulerian approach. The grid sizes of TP2D and FreeLIFE numerical benchmarks were $h = 1/320$ and $h = 1/160$, respectively with corresponding time steps as $h/16$ and $h/2$. Štrubelj *et al* [11] uses an improved two fluid model with interface sharpened by conservative level set method. Klostermann *et al* [11] carried out numerical simulation for benchmark cases 1 and 2 using VOF approach implemented in OpenFOAM version 1.5.1. The grid size used by Klostermann *et al* [11] was $h = 1/320$ with time step of $h/2$.

Towards verification of the interFoam solver with present discretization schemes, the benchmark cases 1 and 2 are studied using four different mesh sizes, $h = 1/40$, $1/80$, $1/160$ and $1/320$. The simulation time is $t_{final} = 3$ s with a grid size dependent time step of $\Delta t = h/16$ as shown in table 2. The computing times for both test cases are also presented in table 2 for better understanding of computing performance for the operating system used. The bubble profile for the benchmark case 2 at $t = 3$ s is predicted by the present study and is compared in figure 2 with the shapes calculated by earlier authors [27]. The shape is quite similar but from the visual qualitative comparison it is not possible to conclude the correctness of the solution. Hence, verification of the present study simulations is carried out for quantitative parameters such as bubble rise velocity and center of mass position.

Figure 3 shows the verification of temporal variation of rise velocity and center of mass position for benchmark cases 1 and 2. The results of the VOF simulations for the four mesh sizes, $h = 1/40$, $1/80$, $1/160$ and $1/320$ are compared with the corresponding benchmark results predicted by the TP2D, FreeLIFE and MooNMD codes [28] and benchmarks of Hysing *et al* [27], Štrubelj *et al* [11] and Klostermann *et al* [11]. The verification of present study predicted results with earlier predictions in literature for benchmark case 1 is presented in table 3. The percentage deviation of the present study for $h = 1/320$ compared with the benchmark data [27] are around 1% for final position of center of mass at $t = 3$ s, 5% for incidence time of

Table 1. Fluid properties for two benchmark validation cases.

Case	ρ_1 (kg/m ³)	ρ_2 (kg/m ³)	μ_1 (Pa.s)	μ_2 (Pa.s)	σ (N/m)	g (m/s ²)
1	1000	100	10	1	24.5	0.98
2	1000	1	10	0.1	1.96	0.98

Table 2. Grid refinement $1/h$, number of elements, time step and computation time using present study for benchmark validation cases.

$1/h$	$n_{elements}$	Δt , s	Computation time case 1	Computation time case 2
40	3200	1.5×10^{-3}	3.5 minutes	3.7 minutes
80	12800	7.8×10^{-4}	52 minutes	1.7 hour
160	51200	3.9×10^{-4}	13.5 hour	10.1 hour
320	204800	1.9×10^{-4}	13 days	12 days

Figure 2. Verification of present study bubble profile with earlier predictions for benchmark case 2 at $t = 3$ s.

Figure 3. Verification of present study predicted center of mass position and rise velocity (**top**) case 1 (**bottom**) case 2.

maximum velocity ($u_{\max}$) and 3% for $u_{\max}$. However, the percentage deviation of the present study for $h = 1/320$ compared with the OpenFOAM results of Klostermann *et al* [11] are around 1% for all considered parameters for benchmark case 1. For benchmark case 1 with high surface tension, the grid independence is not observed with increase in mesh refinement but the predictions are in close range of the benchmark results.

For benchmark case 2 with lower surface tension, increase in mesh refinement, resulted in predictions close enough to benchmark results of FreeLIFE code as shown in figure 3 and table 4. The percentage deviation of the present study for $h = 1/320$ compared with the benchmark data of FreeLIFE [28] are around 1% for final position of center of mass at $t = 3$ s and incidence time of second maximum velocity ($u_{\max 2}$), 3% for incidence time of first maximum velocity ($u_{\max 1}$) and $u_{\max 1}$ and 4% for $u_{\max 2}$. However, the percentage deviation of the present study for $h = 1/320$ as compared to the OpenFOAM results of Klostermann *et al* [11] are around 1% for all considered parameters except incidence time of $u_{\max 1}$, which is around 5% for benchmark case 2. The verification studies showed that the VOF solver used in the present study is able to predict the benchmark results for bubble rise for both low and high surface tension fluids.

4.2 Experimental validation of solver

The experimental validation of solver is carried out with experimental correlations [29] available in literature for bubble terminal velocity. Figure 4 shows the validation of Froude number $\left(Fr = \frac{U_T}{\sqrt{g d_B}}\right)$ for air-water system as a function of bubble diameter to domain width ratio $\left(\frac{d_B}{W}\right)$. Validation is carried out for an air bubble diameter of 20 mm rising in water column for bubble diameter to domain width ratios of 0.125 and 0.4. A good comparison is

Table 3. Verification of present study with benchmark results for high surface tension case 1.

	Maximum rise velocity		center of mass position (m) at $t = 3$ s
	t (s)	$u_{\max}$ (m/s)	
present study ($1/h = 40$)	0.941	0.236	1.062
present study ($1/h = 80$)	0.938	0.236	1.063
present study ($1/h = 160$)	0.944	0.237	1.065
present study ($1/h = 320$)	0.967	0.236	1.069
TP2D	0.921	0.242	1.081
FreeLIFE	0.931	0.242	1.080
MooNMD	0.924	0.242	1.081
Hysing <i>et al</i>	0.927	0.242	1.081
Štrubelj <i>et al</i>	0.924	0.246	1.068
Klostermann <i>et al</i>	0.952	0.235	1.070

Table 4. Verification of present study with benchmark results for low surface tension case 2.

	Maximum rise velocity				center of mass position (m) at $t = 3$ s
	t (s)	$u_{\max 1}$ (m/s)	t (s)	$u_{\max 2}$ (m/s)	
present study ($1/h = 40$)	0.767	0.249	1.706	0.218	1.099
present study ($1/h = 80$)	0.753	0.245	1.872	0.225	1.104
present study ($1/h = 160$)	0.746	0.242	1.953	0.230	1.111
present study ($1/h = 320$)	0.749	0.244	2.003	0.234	1.119
TP2D	0.733	0.252	2.07	0.243	1.138
FreeLIFE	0.728	0.251	1.984	0.244	1.125
MooNMD	0.732	0.250	2.06	0.239	1.139
Klostermann <i>et al</i>	0.716	0.247	2.005	0.235	1.122

obtained between the numerical prediction and experimental correlation as shown in figure 4, confirming the validation of interFoam solver for present study.

5. Grid independence

A grid independence study is carried out to find the grid size required for simulating an initially static spherical bubble that rises in a quiescent liquid sodium pool. Argon gas bubble of initial diameter 20 mm is considered for the study. The domain width and height considered for the study is 160 mm. The thermo physical properties of argon (Ar) and sodium (Na) are evaluated at 473 K. The grid independence for the present system is carried out by simulating the case for three grid sizes 512×512 (coarse), 544×544 (medium) and 576×576 (fine). The results of the study for various grid sizes are compared in figure 5. Figures 5(a) and 5(b) showed that average bubble rise velocity and center of mass position are almost same for all three grid sizes studied. Hence, domain with grid size of 544×544 is chosen for the present study considering the grid independence achieved and higher computational cost involved in finer mesh studies. The computational time required for simulating a grid size of 544×544 is 4 days.

6. Results and discussion

The numerical simulation of inert gas bubble dynamics in liquid sodium/NaK pool is studied parametrically to understand the effect of bubble size, domain aspect ratios and gas-liquid components. The sensitivity studies are

Figure 4. Validation of interFoam solver for bubble terminal velocity in air-water system.

carried out considering 20 mm bubble diameter as the base case for the range of bubble sizes typical to SFR for source term evaluation [16, 17]. The evaluation is classified into the following sections.

6.1 Effect of bubble size

The bubble rising behavior is size dependent and its shape is related to the following dimensionless parameters.

Morton number which depends on fluid properties is given by:

$$Mo = \frac{g\mu_l^4}{\rho_l\sigma^3} \quad (13)$$

The Eötvös number, which represents the ratio of gravitational to surface tension force, is given by:

$$Eo = \frac{g\rho_l d_B^2}{\sigma} \quad (14)$$

The Reynolds number, which represents the ratio of inertial to viscous force, is given by:

$$Re = \frac{d_B U_T \rho_l}{\mu_l} \quad (15)$$

The Capillary number, which represents the ratio of viscous to surface tension force, is given by:

$$Ca = \frac{\mu_l U_T}{\sigma} \quad (16)$$

Numerical simulations are carried out to understand the effect of initial bubble diameter on bubble dynamics for argon gas and liquid sodium system at 473 K. The domain height ‘ H ’ and width ‘ W ’ are taken as “ $8 d_B$ ” so that the bubble reaches terminal velocity and side wall effects can be ignored [12]. The different bubble diameters considered for the analysis are 10 mm, 15 mm and 20 mm. The non-dimensional parameters for bubble dynamics are evaluated from the characteristic bubble velocity [11], $U_T = \sqrt{gd_B}$ as shown in table 5.

The simulation results of bubble rising trajectories and shapes in the liquid sodium for different bubble sizes are depicted in figure 6. The rise time, number of elements and computing time for various bubble diameters in the present study are given in table 6. Figures 6(a)-(c) show that for the

Figure 5. Grid independence study cases with different mesh sizes for (a) average rise velocity with rise height (b) center of mass position with time for rising bubble.

Table 5. Bubble conditions for argon-sodium system.

d_B (mm)	Mo	Re	Eo	Ca
10	6.7×10^{-14}	6262.0	4.7	7.5×10^{-4}
15	6.7×10^{-14}	11505.7	10.6	9.1×10^{-4}
20	6.7×10^{-14}	17714.0	18.8	1.1×10^{-3}

range of bubble sizes studied, 20 mm bubble movement is relatively stable and its rising trajectory is almost rectilinear. The temporal variation of bubble dynamic parameters and rise trajectory for center of mass position of bubble diameters ranging from 10 to 20 mm are shown in figures 7 and 8. Figure 7 shows that the bubble rise velocity reaches 0.2 m/s in 0.104 s, 0.062 s and 0.025 s for 10 mm, 15 mm and 20 mm bubble, respectively.

The oscillations in the bubble vertical velocity component are seen and are due to the influence of horizontal velocity components (figure 7). The oscillations are found to be more pronounced for lower bubble sizes and the amplitude is observed to decrease with increase in bubble diameter. The maximum deviations in rise velocities for 10 mm and 15 mm bubble sizes from 20 mm case are observed to decrease with increase in bubble diameter. It can be seen that the maximum deviations in rise velocity of 10 mm and 15 mm from the 20 mm bubble case are 31.6% and 28.1%, respectively as shown in figure 7.

The deviation from rectilinear motion is least for 20 mm, with a maximum deviation of 0.0009 m from the central axis at 0.425 s as shown in figure 8(a). Figure 8(a) signifies that the bubble rise becomes rectilinear for argon-sodium system at a diameter of 20 mm. The maximum horizontal

Figure 6. Bubble rising trajectories for (a) 10 mm, (b) 15 mm and (c) 20 mm.

Table 6. Number of elements and computation time for argon-sodium system with Aspect Ratio (AR) = 1.

d_B (mm)	Rise time (s)	$n_{elements}$	Computation time
10	0.225	295936	4 days
15	0.350	295936	4 days
20	0.425	295936	4 days

Figure 7. Temporal variation of rise velocity for various bubble diameters in argon-sodium system.

deviations from the central axis are also given in table 7. It can be seen that the deviation for 20 mm is 1.14% of the half width of the domain cavity. Since, the horizontal deviation from central axis is least for 20 mm bubble; its

Table 7. Maximum horizontal deviation from central axis for argon-sodium system with $AR = 1$.

d_B (mm)	Maximum horizontal deviation from central axis (m)	% of horizontal deviation w.r.t half width of domain cavity
10	9.8×10^{-4}	2.5
15	6.2×10^{-3}	10.3
20	9.1×10^{-4}	1.1

rise trajectory is rectilinear compared to 10 mm and 15 mm bubbles sizes. Figure 8(b) shows the temporal variation of center of mass position for bubble sizes 10 mm, 15 mm and 20 mm. The initial offset at time, $t = 0$ s is due to the differences in initial sizes and elevation. Figure 8(b) shows that at 0.225 s, the 20 mm bubble travels vertically 0.047 m. At $t = 0.225$ s, the distance travelled vertically by 10 mm bubble is lower than that of 20 mm bubble by 12.14% due its lower rise velocity. The average bubble terminal velocity is found to be 0.21 m/s for bubble diameters ranging from 10 to 20 mm. The highest value of bubble terminal velocity is 0.24 m/s for 20 mm bubble and the lowest is 0.18 m/s for 10 mm bubble as shown in figure 9.

6.2 Effect of domain aspect ratio

Simulations are carried out to understand the effect of domain Aspect Ratio (AR) on bubble dynamics for argon-sodium system. The influence of AR on bubble dynamics is

Figure 8. (a) Lateral position of center of mass, (b) Axial position of center of mass with time for argon-sodium system.

studied in detail by varying the domain height and width independently.

6.2a Effect of domain height: The aspect ratio is varied by changing the height of the domain for a fixed domain width of 160 mm. The three different domain aspect ratios considered for the analysis are 1, 1.25 and 1.5 for a fixed bubble diameter of 20 mm. The temporal variation of bubble dynamics as a function of cavity aspect ratio is given in figures 10 and 11. Figure 10 shows that 20 mm bubble rise velocity reaches 0.2 m/s in 0.025 s for all the aspect ratios studied. The maximum horizontal deviation from the central axis is 4% of the half width of the domain cavity and is insignificant as evident from figure 11(a). Thus, irrespective of the aspect ratio studied, the rise trajectory of the 20 mm bubble is rectilinear. Figure 11(b) also indicates that the rise height for $AR = 1.5$ is less than 1.13% as compared to $AR = 1$ at 0.425 s and hence the deviation is insignificant. The average bubble terminal velocity is 0.23 m/s for aspect ratio of 1 to 1.5 for varying domain height as shown in figure 12. The bubble terminal velocity is found to be 0.238 m/s and 0.235 m/s for $AR = 1$ and 1.5, respectively, the deviation between them being insignificant. The variation of average bubble rise velocity with rise height of 20 mm bubble for varying aspect ratios as a function of domain height are given in figure 13. It is clear that the domain height of $8 d_B$ is sufficient for bubble dynamic simulation in the present study.

6.2b Effect of domain width: Results on the effect of domain width on bubble dynamics for a fixed domain height of 160 mm are presented in this section. The three different domain aspect ratios considered for the analysis are 0.73, 1 and 1.6 for a fixed bubble diameter of 20 mm. The temporal variation of bubble dynamics as a function of

Figure 9. Bubble terminal velocity with bubble diameter for argon-sodium system.

Figure 10. Temporal variation of rise velocity for various domain aspect ratios in argon-sodium system for 20 mm bubble.

cavity aspect ratio is given in figures 14 and 15. Figure 14 shows that 20 mm bubble rise velocity reaches 0.2 m/s in 0.025 s for all the aspect ratios studied. From figure 15(a), the maximum horizontal deviation from the central axis for the ARs studied is 4.2% of the half width of the domain cavity for aspect ratio of 0.73 and the least deviation is 0.75% for aspect ratio of 1.6, which is insignificant. Thus, for aspect ratios of 1 and 1.6, the rise trajectory of the 20 mm bubble is rectilinear. The rise height for the case of $AR = 1$ and 1.6 is 10.1% and 1.9% lower than that for $AR = 0.73$ at 0.425 s as shown in figure 15(b). The average bubble terminal velocity is 0.24 m/s for aspect ratio varying from 0.73–1.6 as shown in figure 16 for varying domain width. The bubble terminal velocity of 0.22 m/s is obtained for $AR = 1.6$, which is 13.6% lower than the bubble terminal velocity of 0.25 m/s for $AR = 0.73$. The variation of average bubble rise velocity with rise height of 20 mm bubble for varying aspect ratios as a function of domain width are given in figure 17. The study confirms that a minimum domain width, $W = 8 d_B$ is to be provided to avoid wall effects as suggested in literature [12].

6.3 Effect of gas-liquid component

Numerical simulations are carried out to understand the effect of various gas-liquid system components on bubble dynamics. The gas-liquid systems considered for the analysis are argon-sodium system at 473 K, xenon (Xe)-sodium system at 820 K and argon-NaK system at 303 K [2, 3]. The domain height ' H ' and width ' W ' are taken as " $8 d_B$ ". The bubble diameter considered for the analysis is 20 mm. The transport properties of the gas-liquid systems considered for analysis are shown in table 8. The bubble dynamics as a function of gas-liquid component is given in

Figure 11. (a) Lateral position of center of mass. (b) Axial position of center of mass with time for 20 mm bubble.

Figure 12. Bubble terminal velocity with domain aspect ratio for 20 mm bubble.

Figure 13. Variation of average bubble rise velocity with rise height for 20 mm bubble.

figures 18 and 19. Figure 18 shows that the bubble rise velocity reaches 0.2 m/s in 0.025 s for all the three gas-liquid systems studied. The maximum deviation in rise velocities for various gas-liquid components from the argon-sodium system case is observed to decrease with increase in surface tension. It can be seen that the rise velocities of xenon-sodium system ($\sigma = 0.155$ N/m) and argon-NaK system ($\sigma = 0.177$ N/m) are lower than argon-sodium system ($\sigma = 0.189$ N/m) by 19% at 0.26 s and 13% at 0.41 s, respectively.

From figure 19(a), the maximum horizontal deviation from the central axis for the gas-liquid component studied is 5% of the half width of the domain cavity for argon-NaK

system. Thus, irrespective of the gas-liquid component studied, the rise trajectory of the 20 mm bubble is rectilinear. Figure 19(b) shows that the maximum bubble rise height is for argon-sodium system at 0.425 s. The rise height for xenon-sodium system is 1.66% lower than that for argon-sodium system and is hence insignificant. Hence, from the parametric study it is clear that the effect of gas-liquid component on bubble dynamics is insignificant for the 20 mm bubble diameter. The average bubble terminal velocity remains almost constant (0.24 m/s) with varying gas-liquid system component as shown in figure 20. The bubble terminal velocity is 0.238 m/s for argon-sodium system and 0.236 m/s for xenon-sodium system, with the deviation being insignificant.

Figure 14. Temporal variation of rise velocity for various domain aspect ratios in argon-sodium system for 20 mm bubble.

Figure 16. Bubble terminal velocity with domain aspect ratio for 20 mm bubble.

6.4 Bubble dynamics in water and sodium

Comparison of bubble dynamics between air-water system and argon-sodium system for 20 mm initial bubble diameter is carried out to understand the similarity between normal liquid and liquid metal single bubble dynamics. The transport properties of fluids used for simulating air-water system and argon-sodium system are shown in table 9. The temporal variations of bubble dynamics for 20 mm air-water and argon-sodium systems are shown in figures 21 and 22. The bubble contour for 20 mm bubble at $t = 0.425$ s is depicted in figure 23, for both air-water and argon-sodium systems.

Figure 21 shows that the rise velocity reaches 0.2 m/s in 0.025 s for both air-water and argon-sodium systems respectively. The maximum deviation in rise velocity for air-water from argon-sodium system is 39% and occurs at 0.135 s due to breakup. The deviation from rectilinear motion is lower for air-water system, with a maximum deviation of 0.0003 m from the central axis at 0.425 s and higher for argon-sodium system, with a maximum deviation of 0.0009 m from the central axis at 0.425 s, as shown in figure 22(a). The maximum horizontal deviation from the central axis for argon-sodium system is 1.14% of the half width of the domain cavity and is insignificant. Thus for both systems the rise trajectory of the 20 mm bubble is rectilinear. Figure 22(b) shows that at 0.425 s

Figure 15. (a) Lateral position of center of mass. (b) Axial position of center of mass with time for 20 mm bubble.

Figure 17. Variation of average bubble rise velocity with rise height for 20 mm bubble.

Table 8. Fluid properties for inert gas-liquid system.

Case	ρ_1 (kg/ m ³)	ρ_2 (kg/ m ³)	μ_1 (Pa.s)	μ_2 (Pa.s)	σ (N/ m)
Argon-sodium ($T = 473$ K)	904	1.04	4.5×10^{-4}	3.2×10^{-5}	0.189
Xenon-sodium ($T = 820$ K)	820	1.97	2.2×10^{-4}	5.6×10^{-5}	0.155
Argon-NaK ($T = 303$ K)	874	1.63	5.3×10^{-4}	2.8×10^{-5}	0.177

the rise height of argon-sodium system are higher than that for air-water system. The rise height for air-water system is 3.03% lower than the rise height for argon-sodium system and is hence insignificant. The bubble terminal velocity of 20 mm bubble in air-water system is 2.23% lower than that for argon-sodium system and is evaluated to be around 0.233 m/s. The bubble dynamic parameters for both the systems are observed to be similar except for the breakup.

Figure 23(a), (b) show that significant breakup to secondary bubbles occurs for the air-water system compared to the argon-sodium system. This suggests that the bubble breakup for liquids with lower surface tension occurs at lower diameters as predicted by Levich correlation [30].

Figure 18. Temporal variation of rise velocity of 20 mm bubble for various gas-liquid systems.

The bubble bottom oscillations are stronger in argon-sodium system than air-water system at 0.425 s as observed by comparing figure 23(a) and f 23(b), respectively. This is due to the higher surface tension of sodium compared to water and is in concurrence with the study of Wang and Tong [9].

7. Conclusions

The interFoam solver of open source CFD package, OpenFOAM version 3.0.0 is used to simulate the rise dynamics of single gas bubble in liquid sodium pool. The VOF module of the solver along with the discretization schemes used in the present study is validated against the numerical benchmark data and experimental results available in literature for single bubble dynamics. The present study investigates the rise dynamics of inert gas bubble in liquid sodium/sodium-potassium alloy (NaK) pool. Parametric studies are carried out to understand the effects of bubble diameter, domain aspect ratio and gas-liquid system on the bubble rise dynamics. The study shows that the bubble rise velocity increases with diameter for liquid sodium systems. The results predict that 20 mm bubble rises rectilinearly and is relatively stable for the range of domain aspect ratios and gas-liquid systems studied. The

Figure 19. (a) Lateral position of center of mass. (b) Axial position of center of mass with time for 20 mm bubble.

Figure 20. Bubble terminal velocity with liquid surface tension for 20 mm bubble.

Figure 21. Simulation results of 20 mm bubble for instantaneous rising velocity of bubble.

bubble dynamics for 20 mm size is observed to be similar in liquid sodium and water systems, except for the lower breakup and higher bottom bubble oscillations characteristics in sodium systems due to higher surface tension. Hence, the present study supports the use of water as a

simulant for sodium systems in bubble dynamic experiments as suggested in literature for SFR source term studies. The study is very useful and forms an intermediate step towards the development of an OpenFOAM based computational framework to analyze heat and mass transfer

Table 9. Fluid properties of 20 mm bubble for air-water and argon-sodium system.

Case	ρ_1 (kg/m ³)	ρ_2 (kg/m ³)	μ_1 (Pa.s)	μ_2 (Pa.s)	σ (N/m)	Mo	Re	Eo
Air-water ($T = 303$ K)	995	1.2	8.0×10^{-4}	1.8×10^{-5}	0.07	1.1×10^{-11}	10953	54.9
Argon-sodium ($T = 473$ K)	904	1.0	4.5×10^{-4}	3.2×10^{-5}	0.19	6.7×10^{-14}	17714	18.8

Figure 22. (a) Lateral position of center of mass. (b) Axial position of center of mass with time for 20 mm bubble.

Figure 23. Bubble contour for 20 mm at $t = 0.425$ s for (a) air-water system, (b) argon-sodium system.

from single bubble rising in liquid sodium pool for reactor safety studies.

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